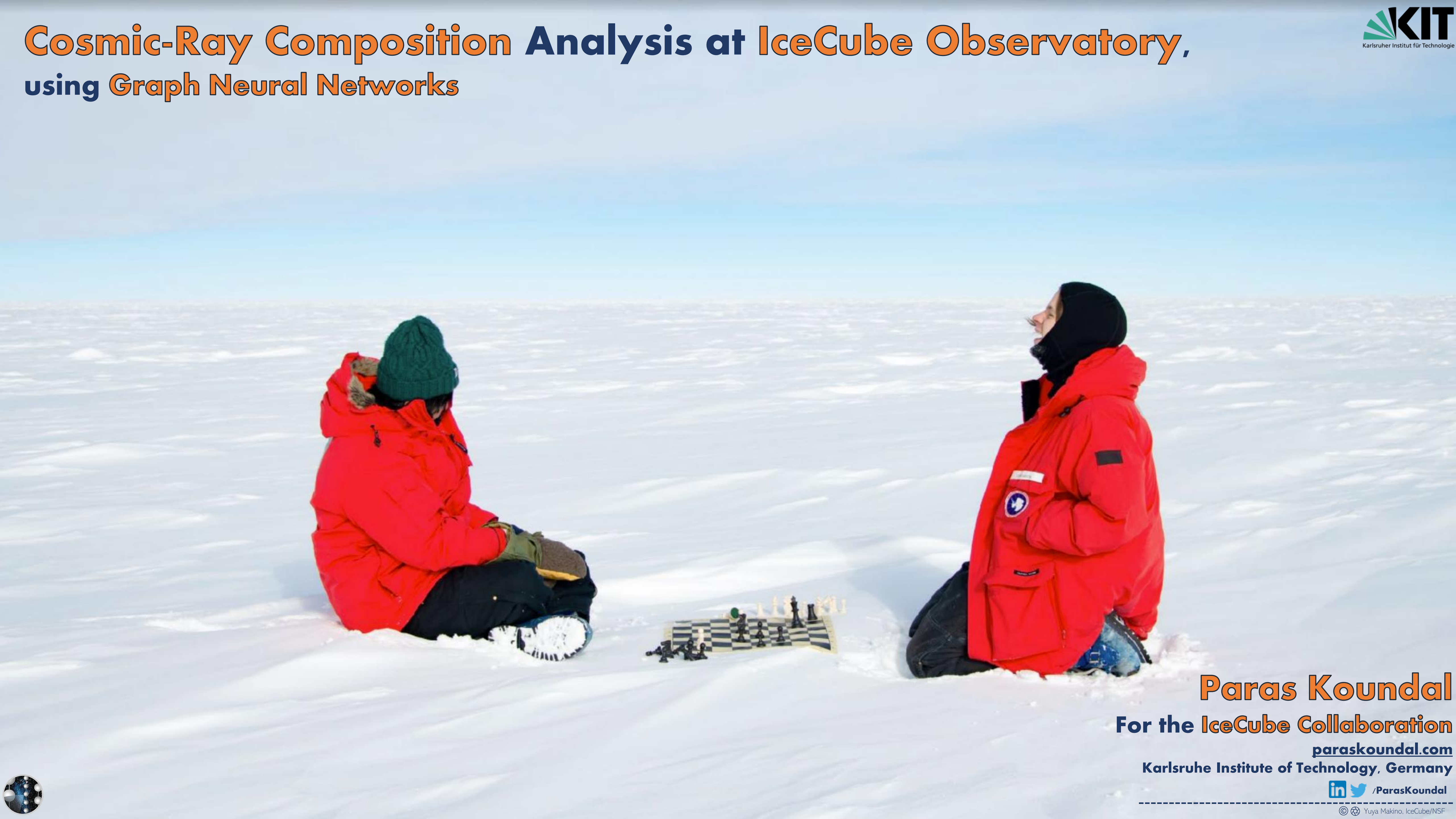


Cosmic-Ray Composition Analysis at IceCube Observatory,

using Graph Neural Networks

Paras Koundal

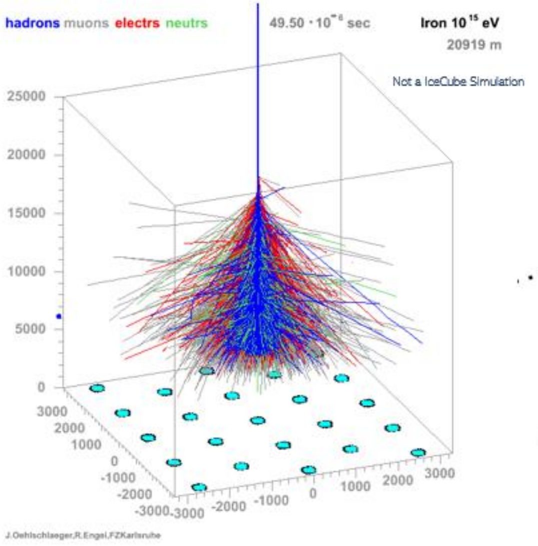
For the IceCube Collaboration

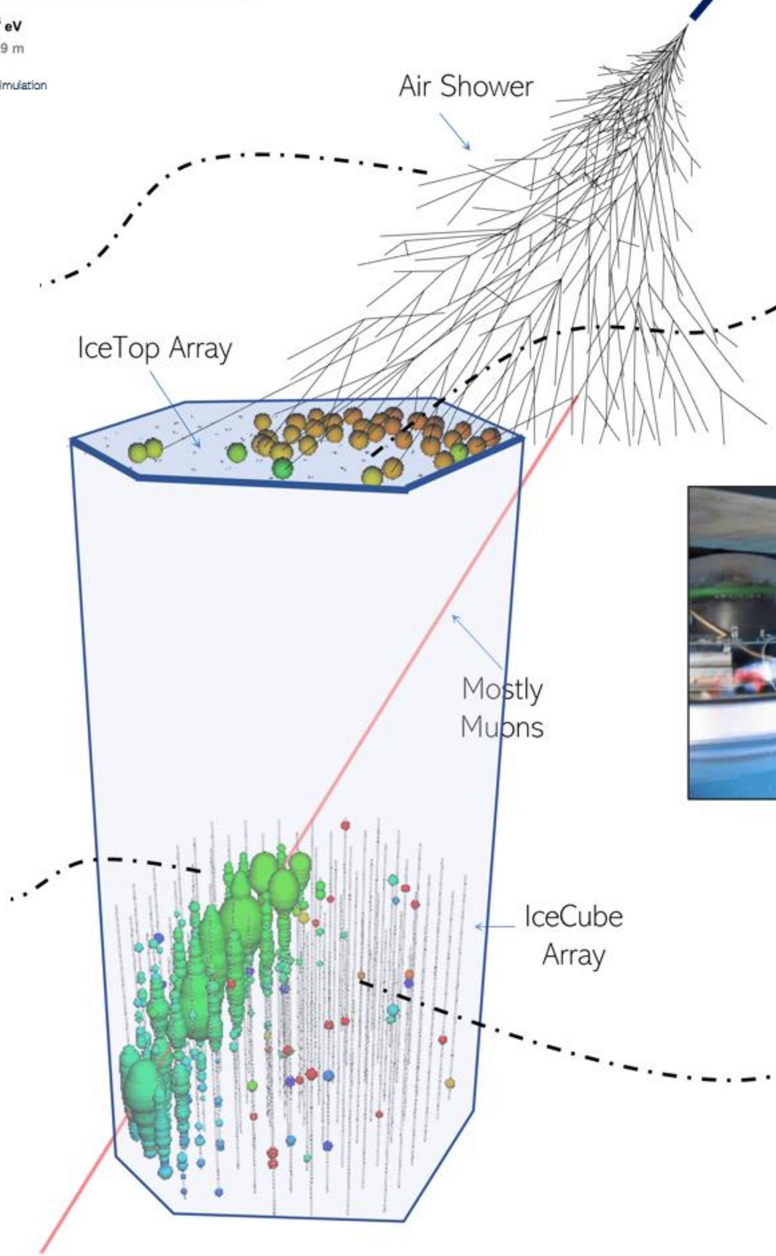
paraskoundal.com

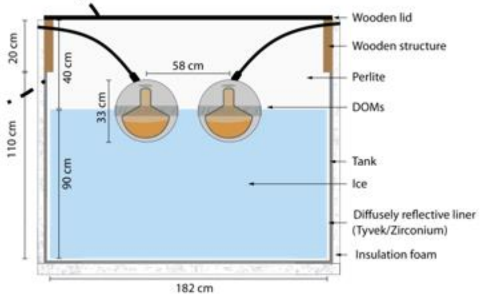
Karlsruhe Institute of Technology, Germany

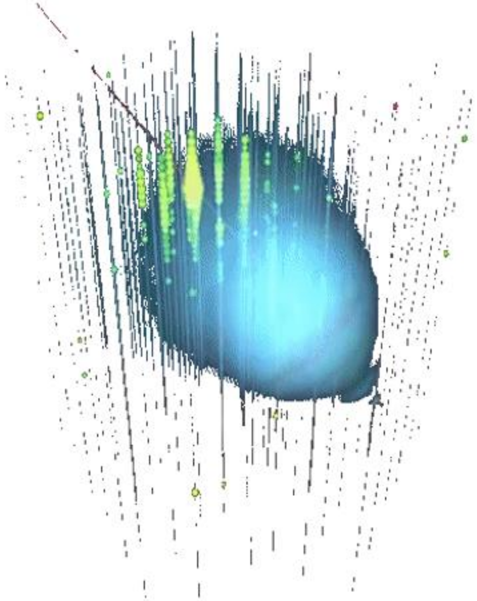
/ParasKoundal

CR Analysis @ IceCube





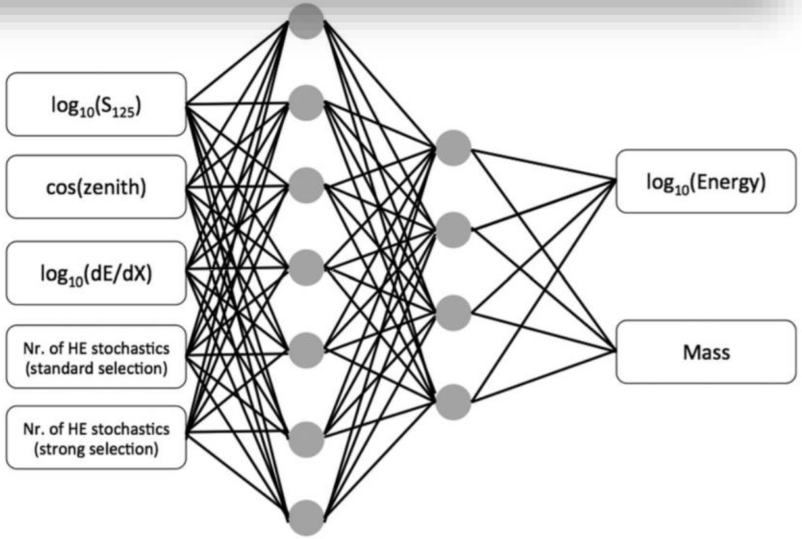




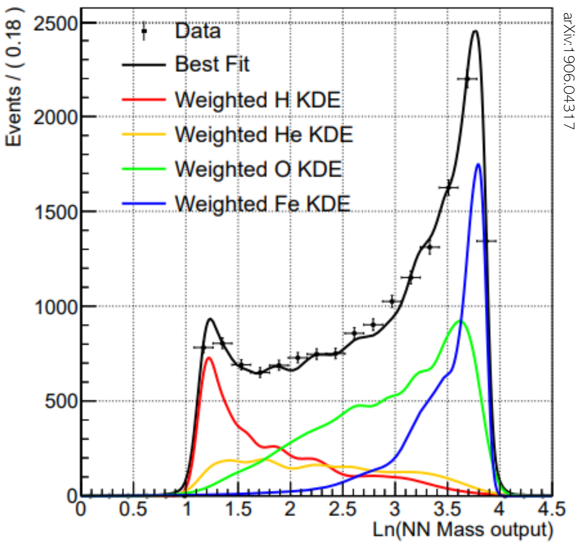
Previous Work

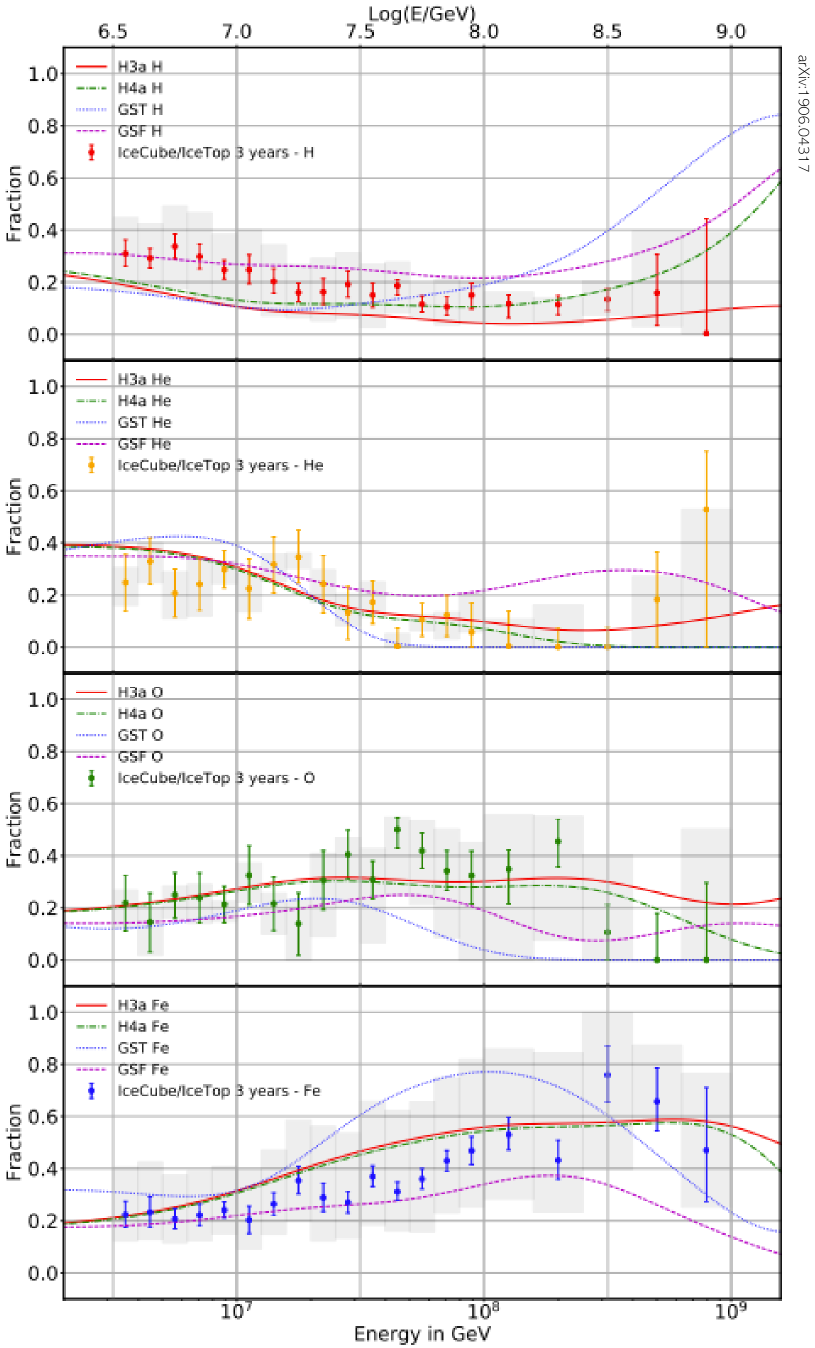
Cosmic ray spectrum and composition from PeV to EeV using 3 years of data from IceTop and IceCube

M. G. Aartsen *et al.* (IceCube Collaboration)
Phys. Rev. D **100**, 082002 – Published 23 October 2019

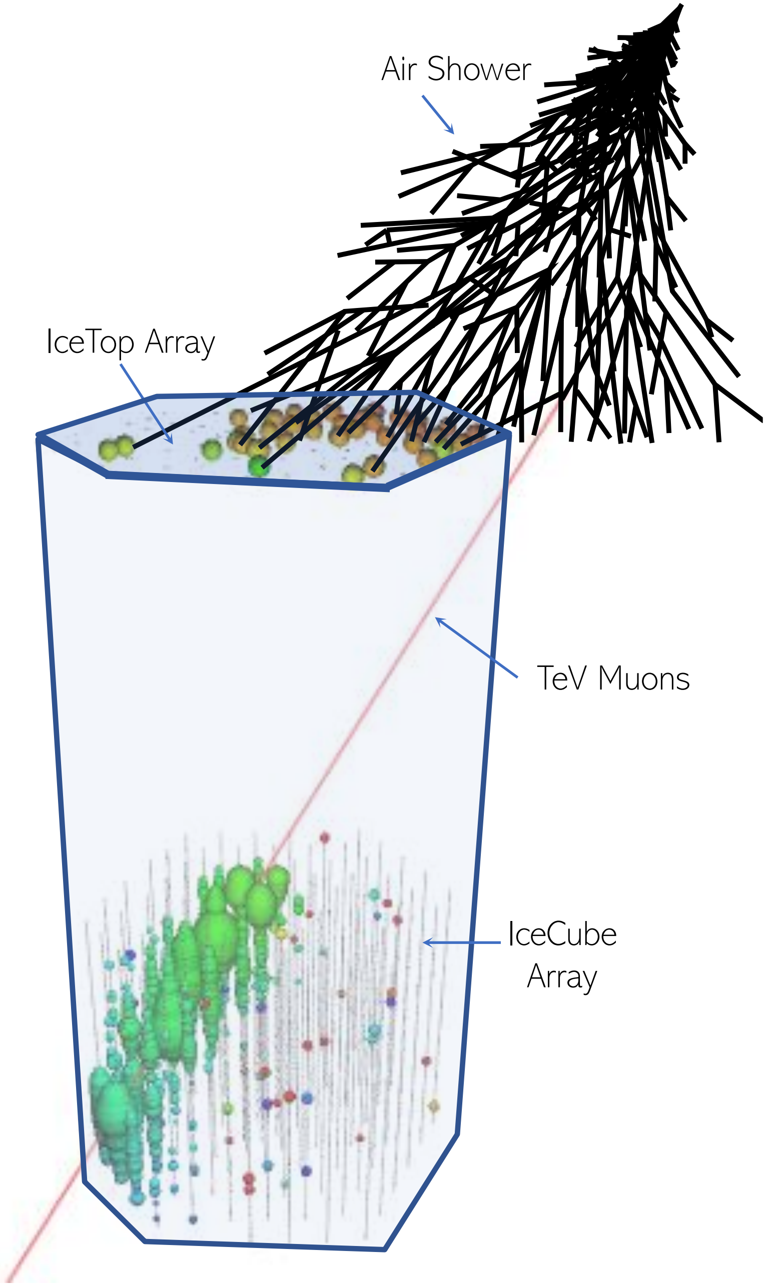


Log(E/GeV): 7.4 - 7.5





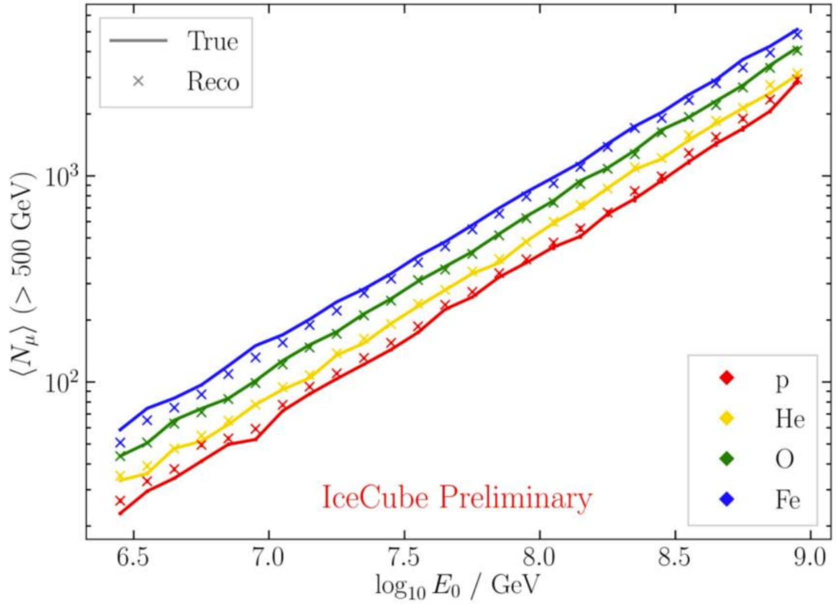
Using Full Signal Footprint



Motivations:

- Benefit from low-level signal information.
  - LDF IceTop and In-Ice
  - Capture H.E. Muon Deposits in-ice
    - For Muon # Estimation – See Stef Verpoest's Work (Jul 28 – Parallel 1)
- Reduce dependence on prior reconstructions
- Faster Inference on real data

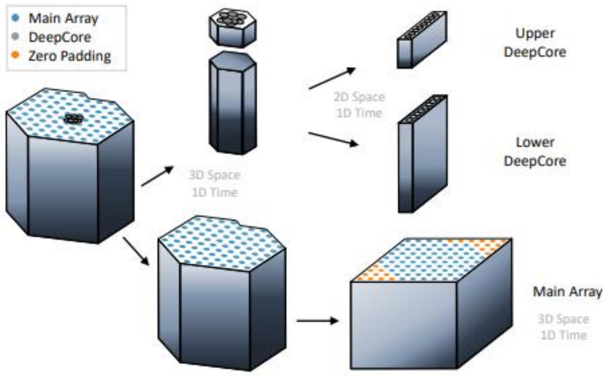
For Details: Stef Verpoest (ECRS22 – Jul 28 [4:45 – Parallel 1])

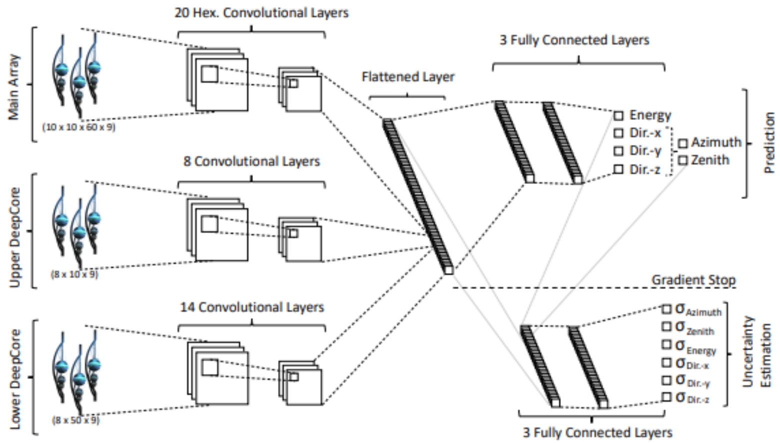


Using In-Ice Signal Footprint

Current Implementation at IceCube

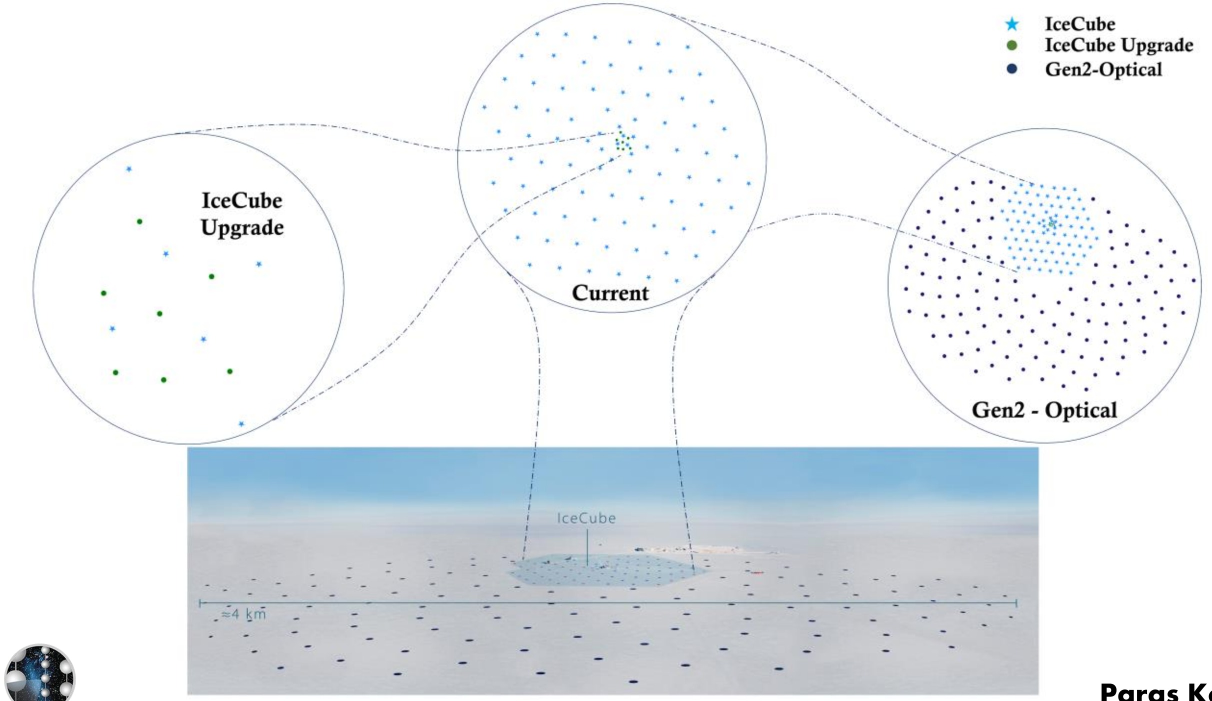
Credits: M. Huennefeld (arXiv:2101.11589)

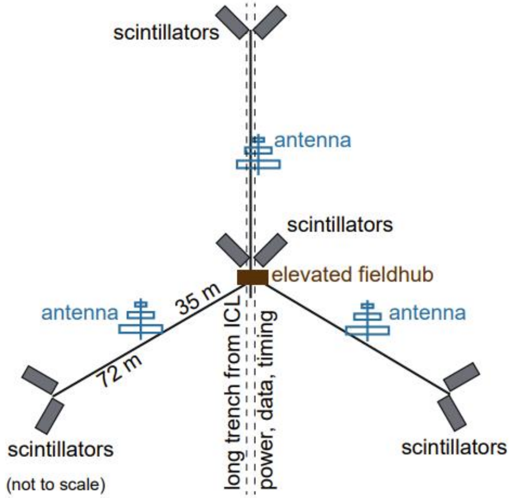


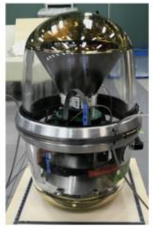


Moving Away from CNNs

Credits: IceCube-Gen2 (arXiv:2008.04323)



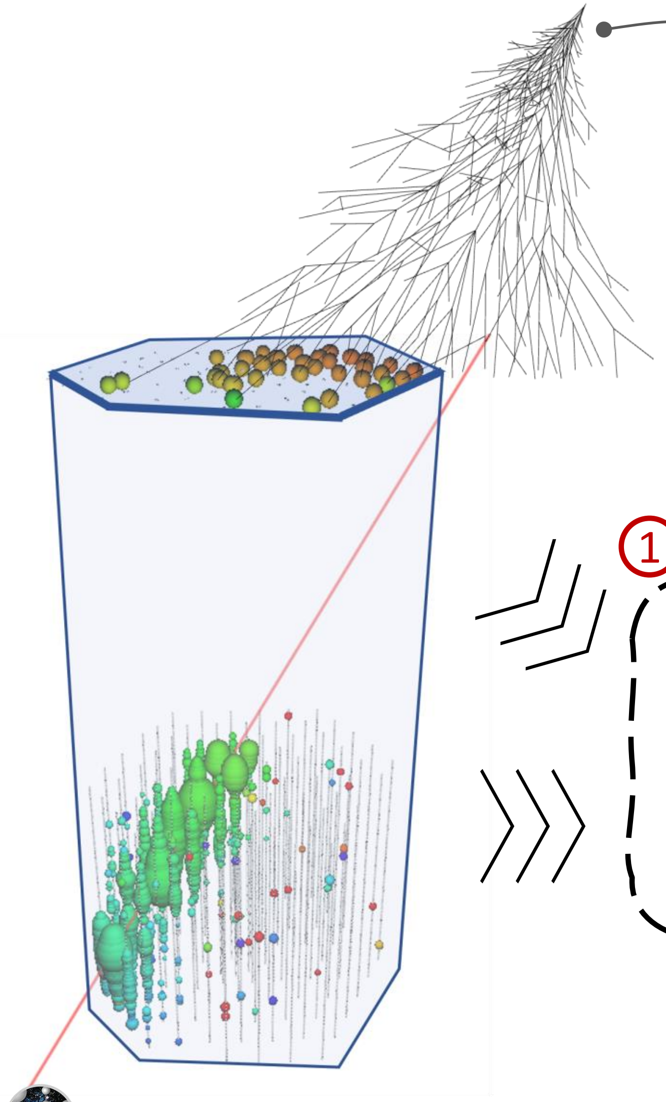




Section 1:

Mass prediction Using GNNs

Learning on Graphs



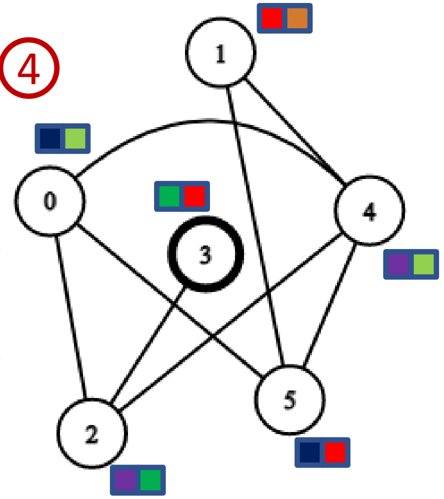
5
Primary Mass Prediction

Input for Graph Neural Network

+

Pre-engineered Features (Mass, Energy & Direction -dependent)

4



1
Spatio-temporal Cleaning of pulses around the track

2
DOMs = Nodes; Node Features = Spatio-temporal measurements ; charge and others

3
Generate Edges between nodes; Weighted kNN

Repeated for Every Event

Feature Info

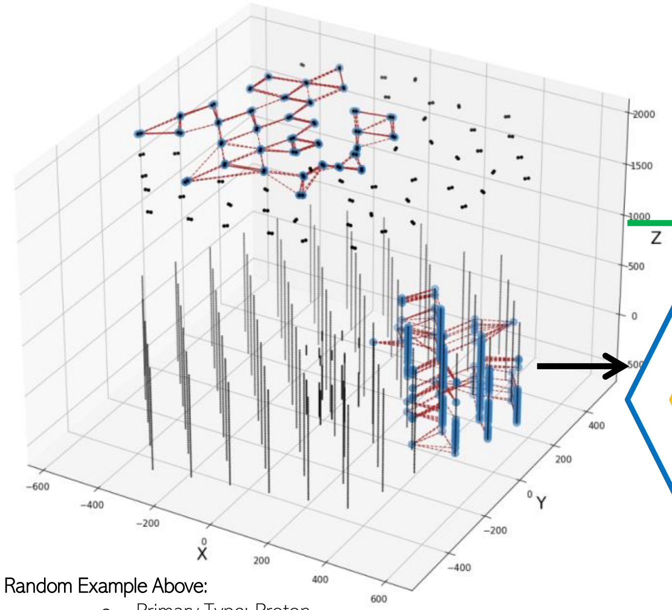
- ## Graph Features
  - Per Node Level
    - Coordinates
    - Charge Deposits
    - Hit-Time
  - Edge Level (For Each Node)
    - k-Nearest Neighbor (Graph-size dependent; Small Graph → Fewer Connections and vice versa)
    - Weighted by Spatial Separation

- ## Pre-engineered Features
  - Primarily Energy Dependent:
    - Shower Size S_{125} (Energy Proxy) [Phys. Rev. D 100, 082002 (2019)]
  - Primarily Composition Dependent:
    - dE/dX_{1500} = Fit value at 1500m of in-ice energy loss profile [Phys. Rev. D 100, 082002 (2019)]
    - Total Stochastic Energy = Energy Deposit by high local stochastic deposits [PoS(ICRC2021)323]
    - Impact Weighted Charge – New
    - Ratio Parameter = Proxy for Muonic to EM Fraction – New
  - Others:
    - Direction: Reconstructed Zenith and Azimuth
    - Slant Length of track in ice
    - Number of Hit DOMs

GNN Architecture

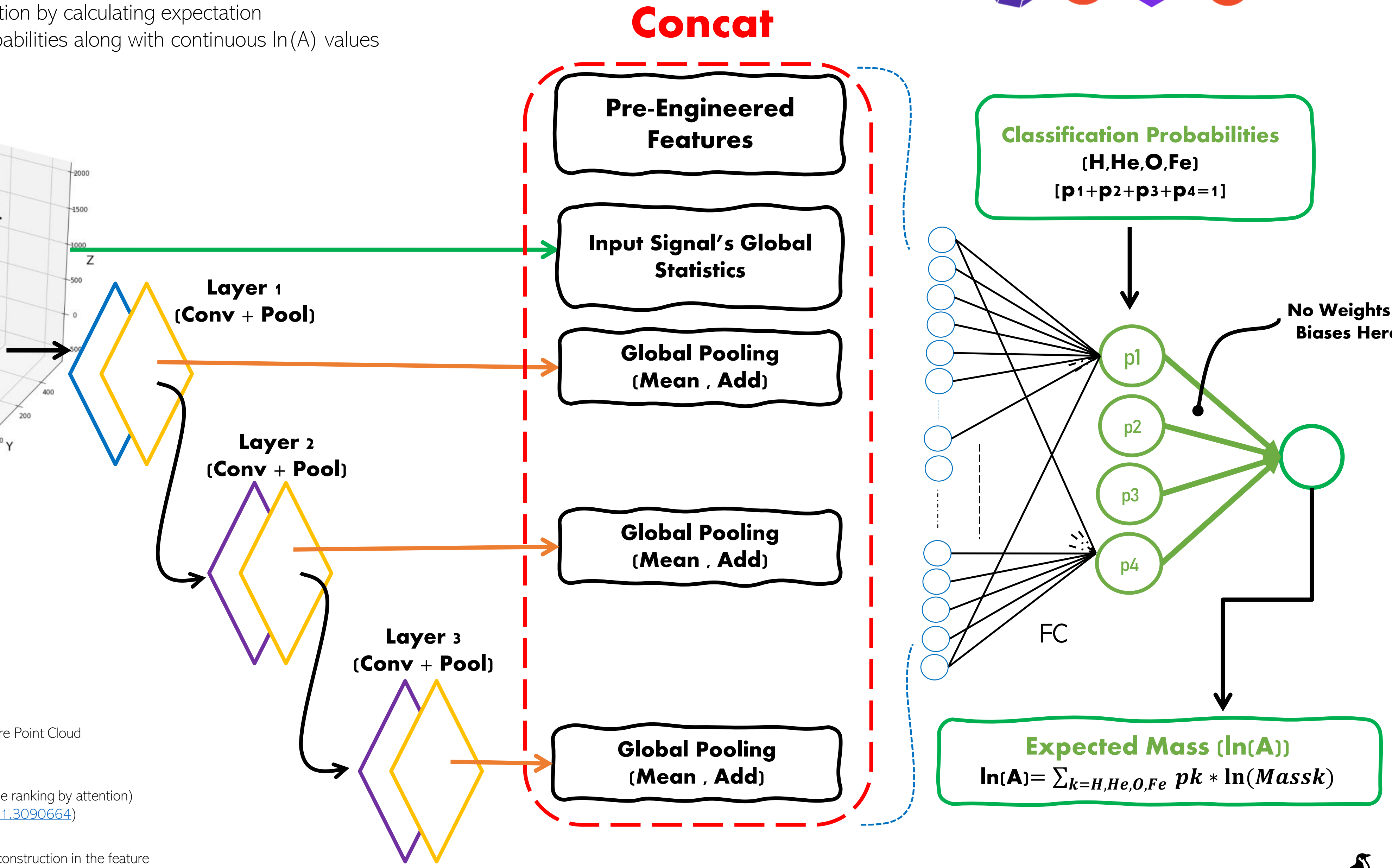
Unique Target Prediction:

- Perform Regression with Classification by calculating expectation
- Allows us to tell element wise probabilities along with continuous ln(A) values



Random Example Above:

- Primary Type: Proton
- Energy ($\log_{10}$/GeV) = 7.28
- Zenith = 17.68 deg
- knn Edges (Weighted), k = 6



Homophily– Measure of Connection between similar nodes (arXiv:2002.05287)

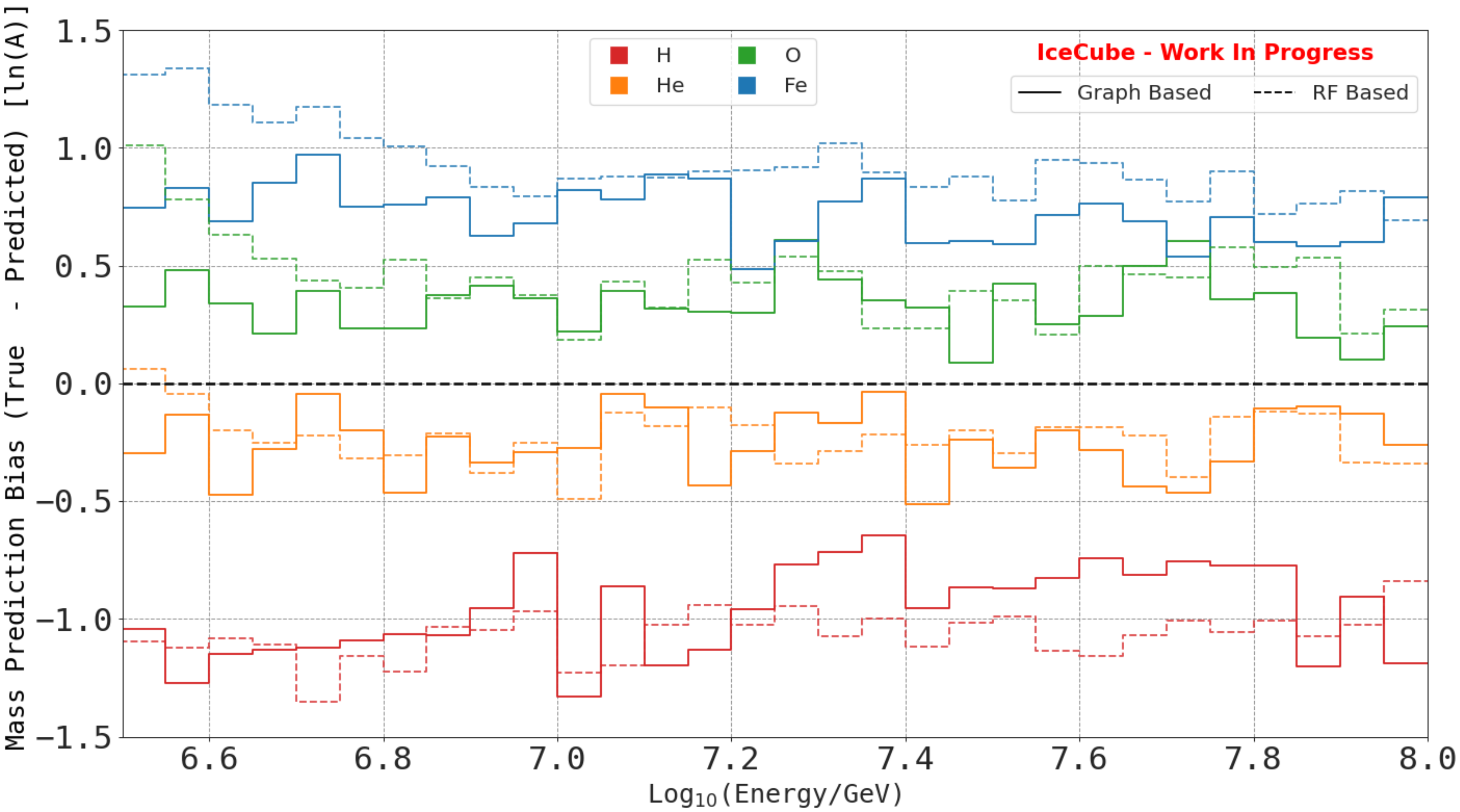
Point-Pair Feature Conv – Global Context Aware Point Cloud Convolution (arXiv:1802.02669)

MVPool – Multi-View Graph Pooling (with node ranking by attention) with Structure Learning (10.1109/TKDE.2021.3090664)

Dynamic Edge Graph Conv – Dynamic Graph construction in the feature space (arXiv:1801.07829)

Results

Mean Bias Reduction For All Primaries in almost all energy bins

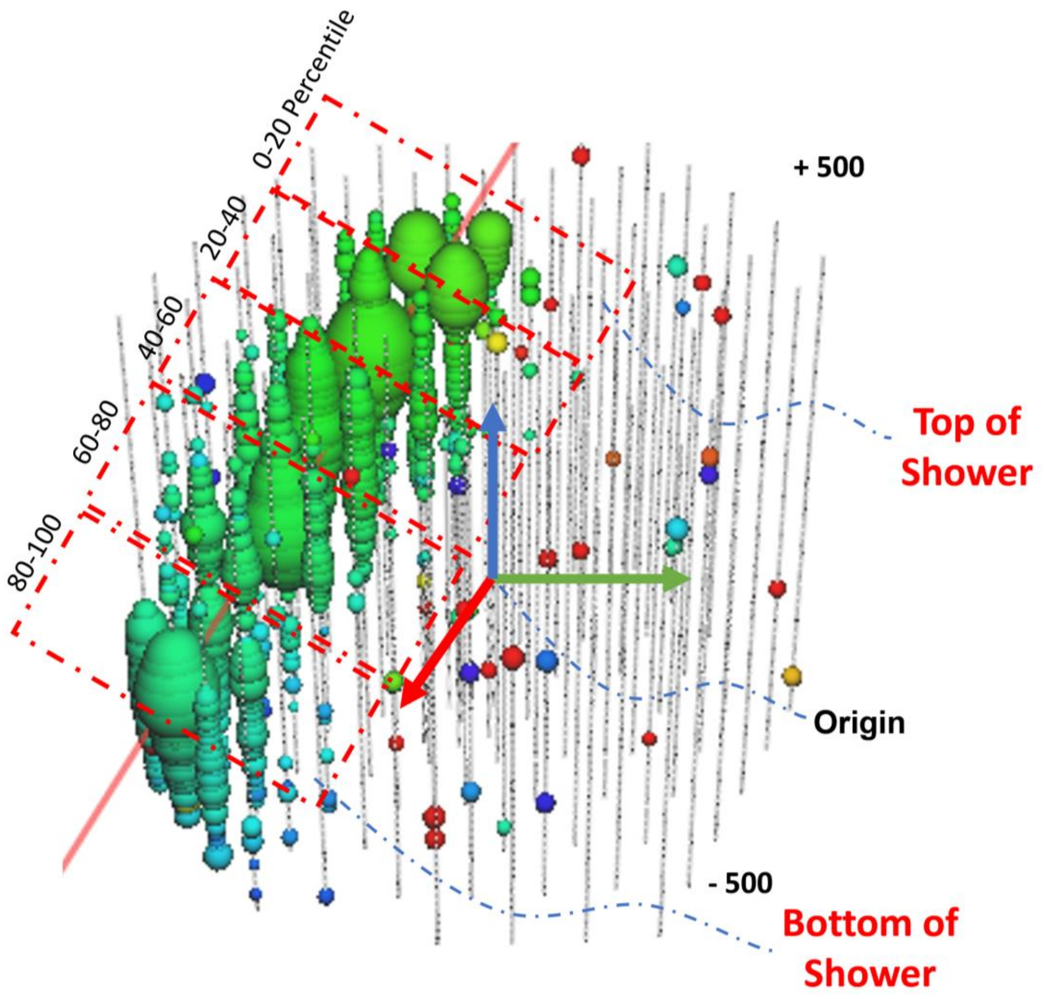


RF Based -[PoS(ICRC2021)323]

Section 2:
Pre-engineered Features

Pre-engineered Features

1. Impact Weighted Charge
   - **Motivation:** At same energy, expect Wider Muon Bundles for Fe than H
   - **Reasons:**
     - Fe-shower interact earlier in the atmosphere
     - Larger Muon Multiplicity → Lower energy muons with larger transversal momenta and are situated further from the shower axis
   - Bin it to observe shower development at different stages
     - Five correlated composition-sensitive parameters
   - Definitions:
     - Impact = Perpendicular distance of each DOM from the track
     - Charge = Charge Deposit at each DOM
     - Percentiles : By number of DOM hits



Impact Weighted Charge

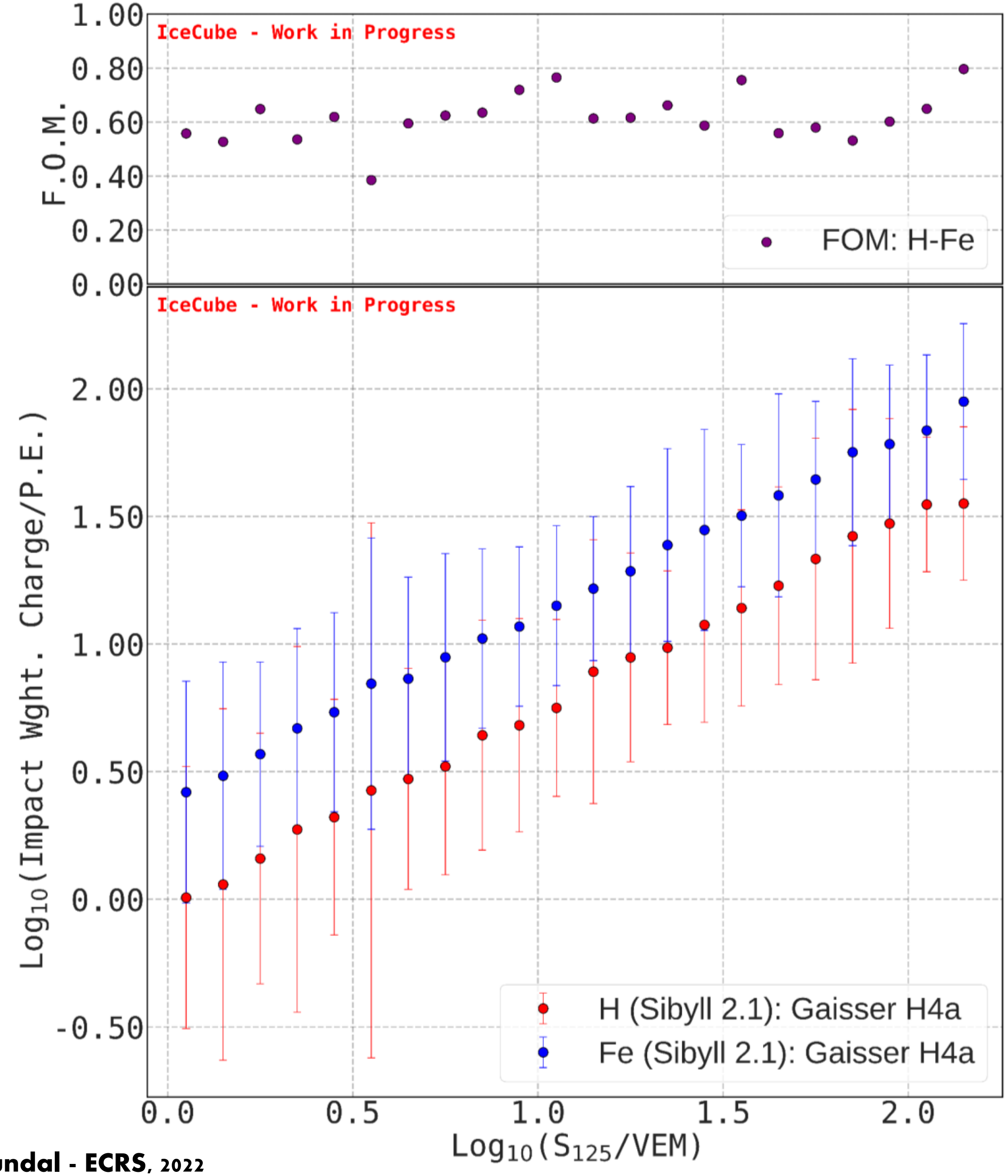
Impact Weighted Charge

(In Each Percentile bin)

$$\frac{\sum Charge_i * ri}{\sum r_i}$$

- **Good Separation Between Primaries**
- Help understand shower attenuation in-ice and a dynamic parameter
- Possibly help in understanding photon propagation in-ice
  - Ongoing work

At Bottom of Shower



Pre-engineered Features

2. Ratio Parameter
   - Motivation: Ratio of Muon to Electron # is a composition sensitive parameter

$$\textbf{Ratio} = \frac{\log_{10} N\mu}{\log_{10} Ne}$$

arXiv:1306.6283

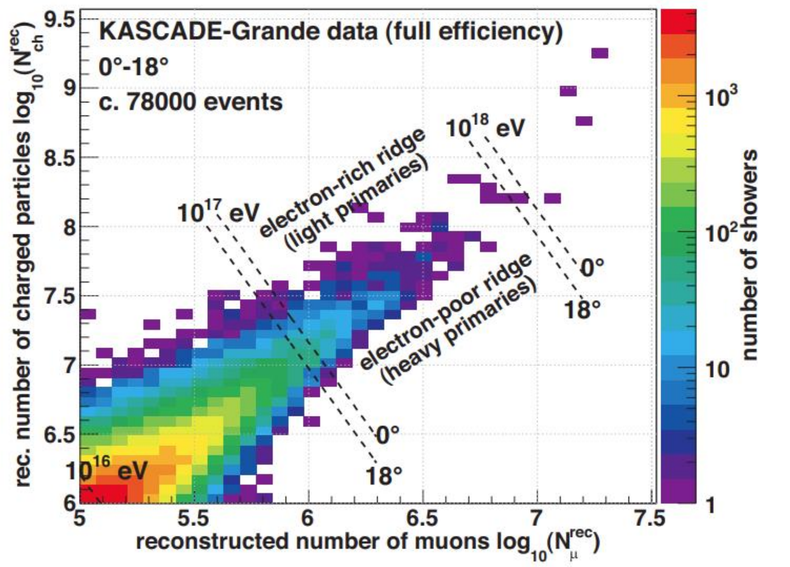


Figure 1: Two-dimensional distribution of the shower sizes (total number of charged particles and of muons) measured with KASCADE-Grande and used for this analysis. Diverse quality cuts are applied. Furthermore, only events with zenith angles $\theta \leq 18°$ and with shower sizes for which the experiment is fully efficient (above $\log_{10}(N_{ch}^{rec}) \approx 6.0$ and $\log_{10}(N_{\mu}^{rec}) \approx 5.0$) are considered. In addition, a roughly estimated energy scale is indicated. Since KASCADE-Grande measures the shower sizes at atmospheric depths beyond the shower maximum, electron-rich showers are initiated preferentially by light primaries, and electron-poor showers by heavy ones, respectively (this is indicated in the figure, too).

$$\frac{\log_{10} N\mu}{\log_{10} Ne}$$

A mass dependent Parameter

Total Energy

$$\textbf{Ratio} = \frac{\log_{10}\mathrm{dEdX}_{1500}}{\log_{10}\mathrm{E}(\mathrm{S}_{125})}$$

$$\log_{10}(E/\mathrm{GeV}) = p_0 + p_1 \log_{10}(S_{125}/\mathrm{VEM}). \quad (2)$$

Using updated simulation and reconstruction algorithms, the mapping of $\log_{10}(S_{125})$ to $\log_{10}(E/\mathrm{GeV})$ from [5] has been re-optimized and applied to the 3-year data set. The updated fit parameters for Eqn. 2 are in the following table:

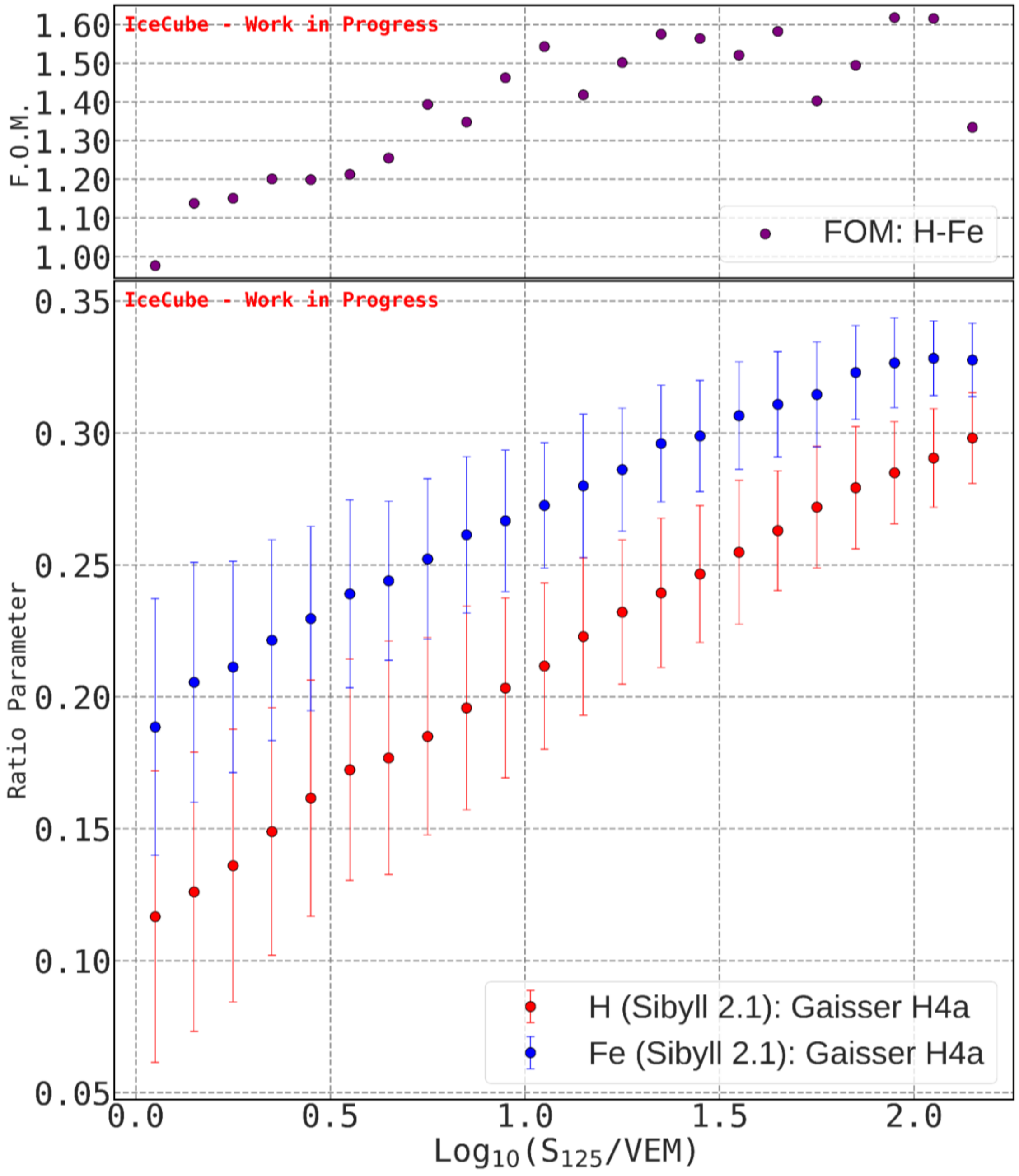
Zenith range	p_0	p_1
$0.95 < \cos(\theta) \leq 1.0$	6.011	0.933
$0.90 < \cos(\theta) \leq 0.95$	6.055	0.924
$0.85 < \cos(\theta) \leq 0.90$	6.110	0.915
$0.80 < \cos(\theta) \leq 0.85$	6.177	0.907

arXiv:1906.04317

Ratio Parameter

$$\textbf{Ratio} = \frac{\log_{10} dEdX_{1500}}{\log_{10} E(S_{125})}$$

- Very Good Separation Between Primaries
- Shows potential benefits of muon & electron number estimate for composition analysis [Related - Stef Verpoest's Work (Jul 28 – Parallel 1)] .



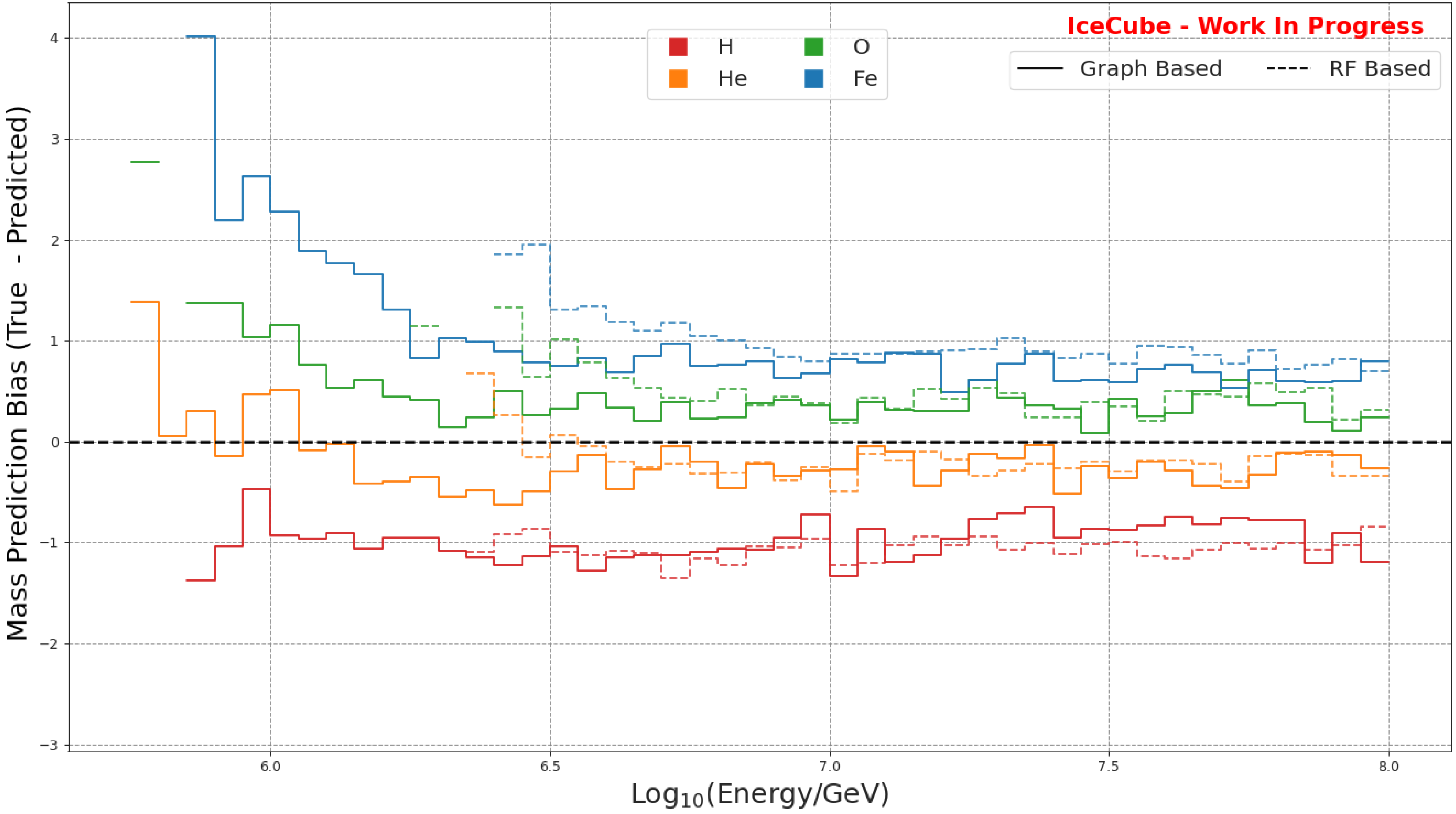
Outlook

- Further improvement by finetuning
- Analysis of Point Probability estimates for each shower
- Comparison with different hadronic interaction models
- Accuracy change by accounting detector effects:
  - Snow-Height changes, DOM Efficiency, scattering and absorption
- Comparisons with Data
  - Individual mass-spectra over the full energy range
  - Mean Mass Spectra
- Energy Spectrum Estimation

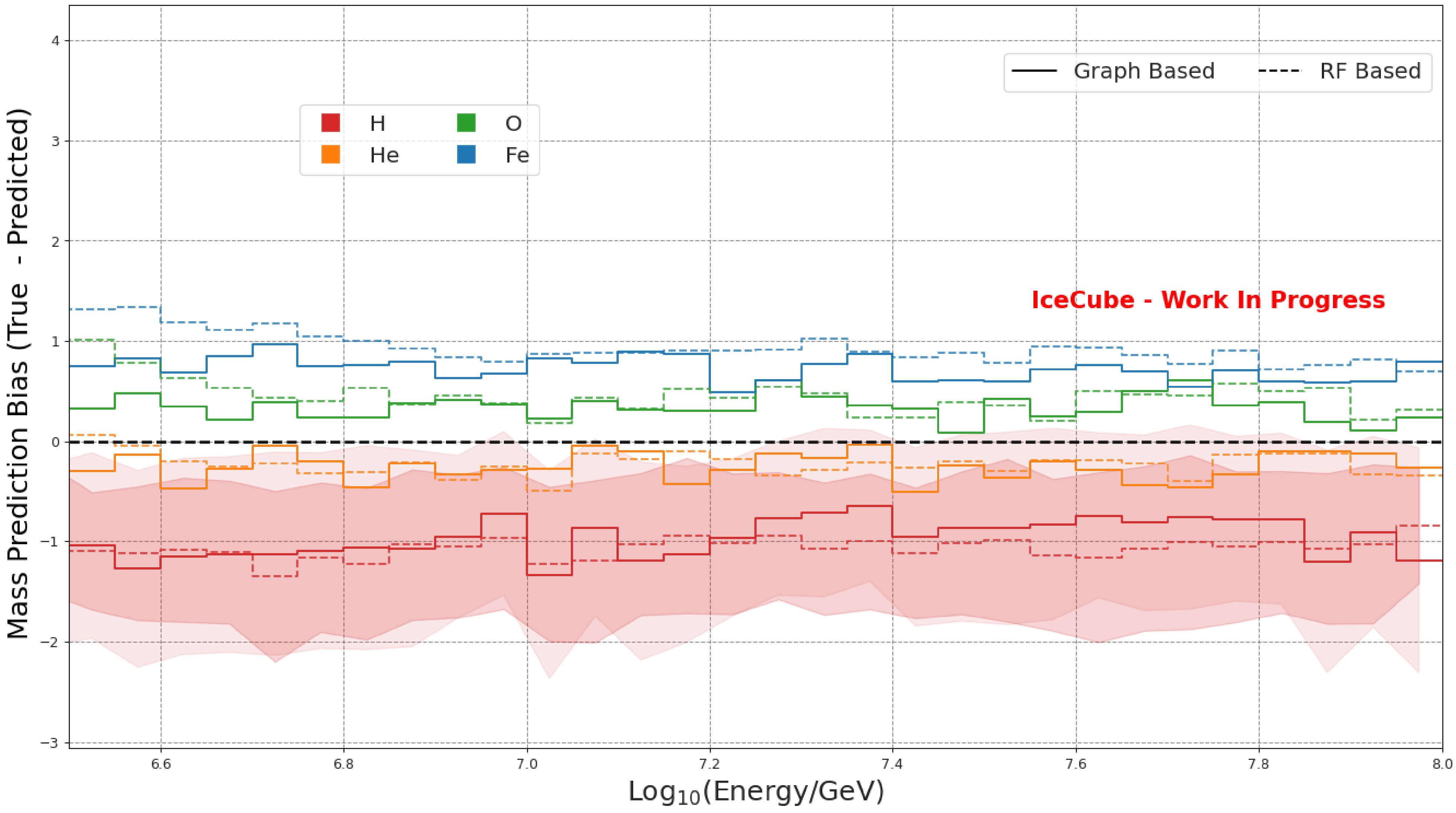
Questions

Results

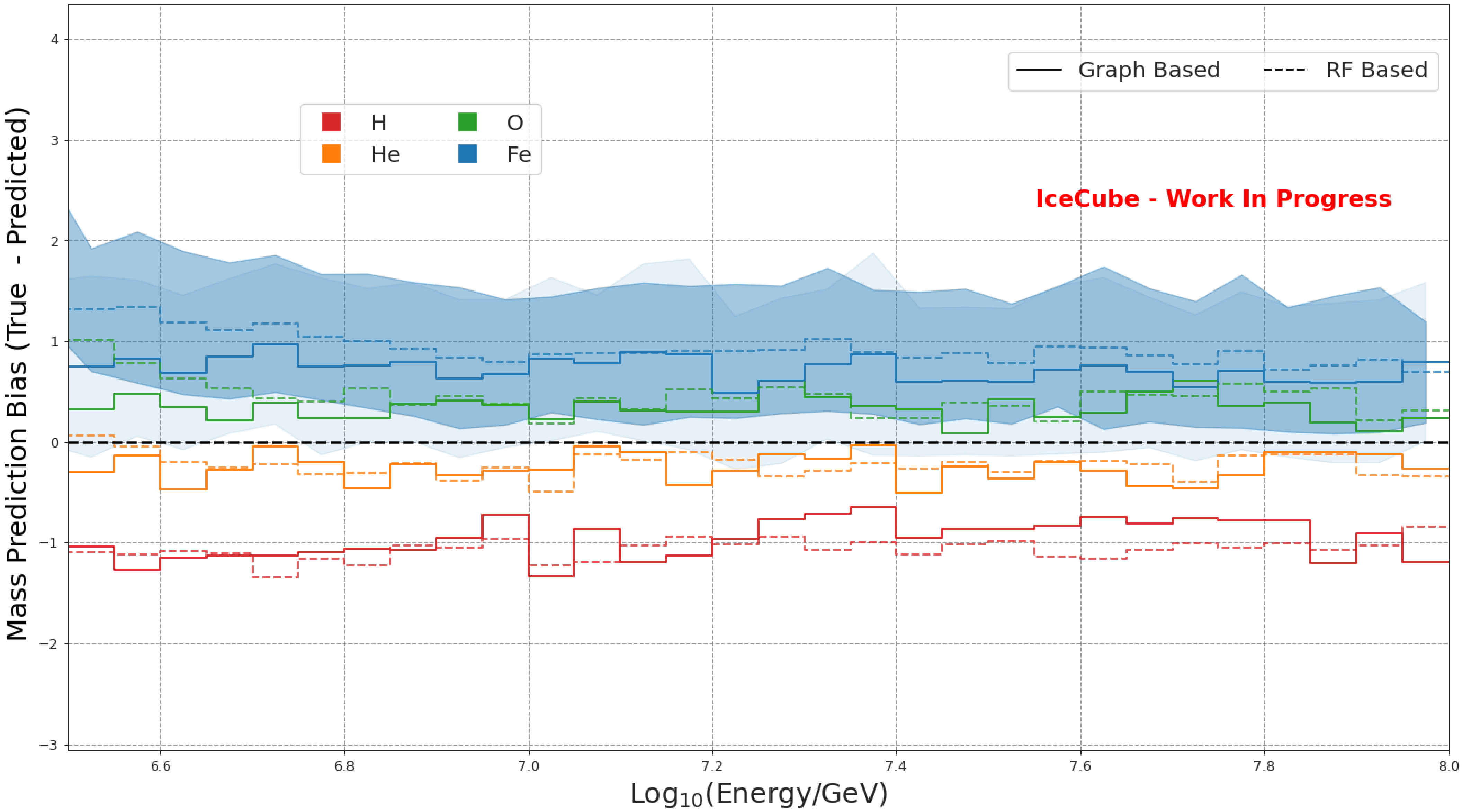
Improvement – Extends beyond



Darker – RF Based ; Lighter – Graph Based



Darker – RF Based ; Lighter – Graph Based



Other Details

Loss = **Classification Loss** + **Regression Loss** + **Embedding Loss (at Concat Layer)**

Hinge Loss

Incorporates loss for distance from the classification boundary into the cost calculation

Smooth L1 Loss

Includes transition between MSE and Absolute Error; less sensitive to outliers

Triplet Margin Loss
(with Cosine Distance)

Measure a relative similarity between samples

Map H-H closer and H-Fe farther; Reduce Dependence on last layer (during backpropagation)

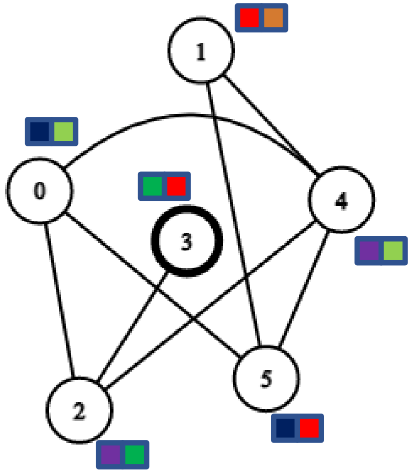
Adam Optimizer; Step on Plateau LR scheduler

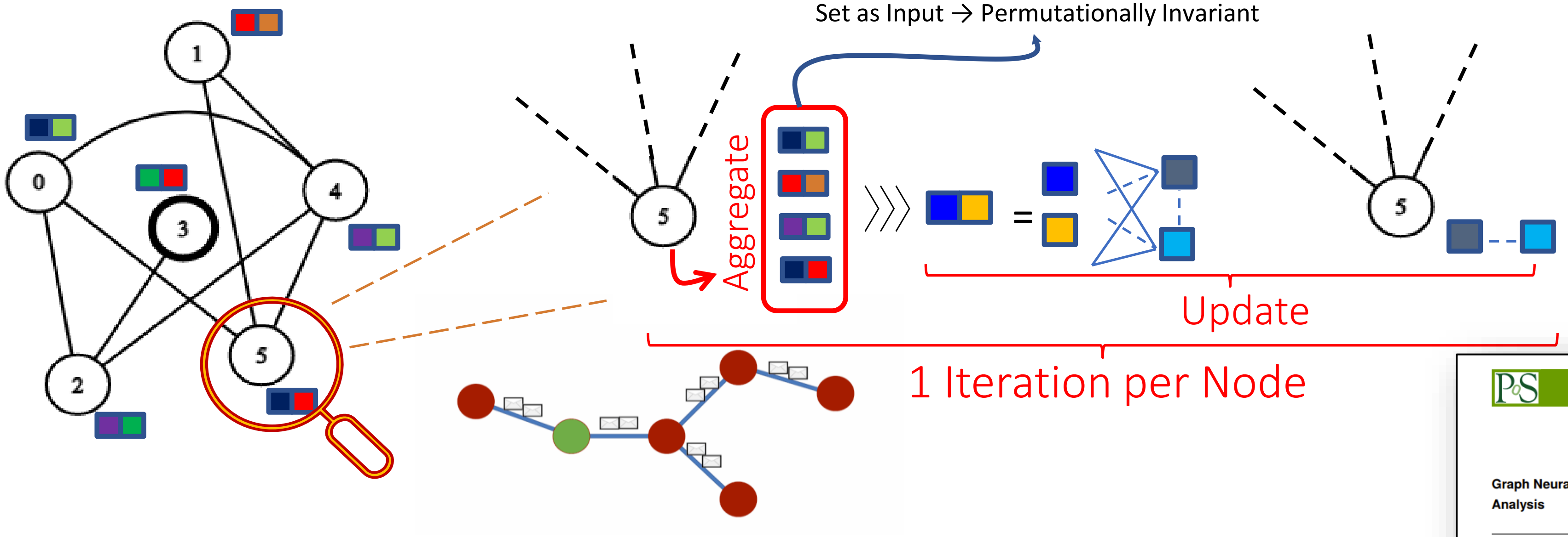
Learning on Graphs

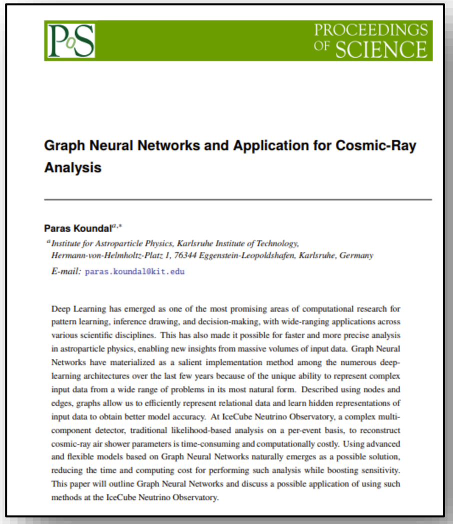
Defined by set of nodes (V) and set of edges (E) between the nodes

- Neighborhood and Connectivity & permutational invariance of Node Labelling

Undirected : Facebook Friends … ; **Directed** : Citation Graph … ; **Bidirectional** : Twitter Follows






PROCEEDINGS OF SCIENCE

Graph Neural Networks and Application for Cosmic-Ray Analysis

Paras Koundal[a,*]

[a] *Institute for Astroparticle Physics, Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Karlsruhe, Germany*

E-mail: paras.koundal@kit.edu

Deep Learning has emerged as one of the most promising areas of computational research for pattern learning, inference drawing, and decision-making, with wide-ranging applications across various scientific disciplines. This has also made it possible for faster and more precise analysis in astroparticle physics, enabling new insights from massive volumes of input data. Graph Neural Networks have materialized as a salient implementation method among the numerous deep-learning architectures over the last few years because of the unique ability to represent complex input data from a wide range of problems in its most natural form. Described using nodes and edges, graphs allow us to efficiently represent relational data and learn hidden representations of input data to obtain better model accuracy. At IceCube Neutrino Observatory, a complex multi-component detector, traditional likelihood-based analysis on a per-event basis, to reconstruct cosmic-ray air shower parameters is time-consuming and computationally costly. Using advanced and flexible models based on Graph Neural Networks naturally emerges as a possible solution, reducing the time and computing cost for performing such analysis while boosting sensitivity. This paper will outline Graph Neural Networks and discuss a possible application of using such methods at the IceCube Neutrino Observatory.

5th International Workshop on Deep Learning in Computational Physics, 2021

Other Material

- paraskoundal.com/dlcp21
- My ML & AI Paper List
- My Twitter (Paras Koundal)